

Photoionization of I^+ ion

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ABSTRACT

Photoionization of the I^+ ion in the energy range of the 4d giant resonance has been studied using our recently developed random-phase approximation with exchange (RPAE) method. Photoionization cross sections for the I^+ $4d - \epsilon f, \epsilon p, 5s - \epsilon p, 5p - \epsilon s, \epsilon d$ have been obtained for each term of the ground state. Calculations include all the intra-shell and inter-shell coupling among the $4d$, $5s$, and $5p$ subshells. Our maximum cross section for the I^+ $4d$ giant resonance, 23.12 MB at 90.24 eV agrees excellently with the recent measurement, 23(3) at 90 eV.

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1 Introduction

Recently, the photoionization of the ion Xe^{q+} ($q=1-6$) [1-9] and the atom I and its ions I^{q+} ($q=1-2$) [10-15], have become "hot topics". Firstly, this is because the 4d giant resonances of the above atom/ions are the important photoionization processes. Secondly, the newly developed RPAE method has made a full RPAE calculation possible for the relevant reactions. Thirdly, the photoionization cross sections for the ionic species are required for plasma modeling.

The random-phase approximation with exchange (RPAE) method has been used to calculate the I^+ photoionization cross section before. However, the calculations [9, 12-13] applied a variety of approximations as the RPAE method was initially developed for the calculation of closed shell atoms only. The previous RPAE calculations referenced above cannot provide the cross sections for each individual term of the I^+ ground state either.

Recently, a RPAE method has been developed by Chen and Msezane [8]. The method has been successfully used to study the inner-shell electron transitions of an atom with an outer open-shell. The calculation can include intra-shell correlations, viz. an electron absorbs a photon then interacts and shares excitation energy with other electrons in the same shell and the inter-shell correlation, where the electron absorbs a photon and interacts and shares the excitation energy with the electrons of the neighboring shells. More recently a RPAE method, which allows for the inclusion of both intra-shell and inter-shell correlations has also been developed by Chen and Msezane for atoms(ions) with an inner open-shell [16]. These methods have greatly extended the scope of the RPAE method as their calculations allow the inclusion of all the inter-shell couplings among the Xe^+ 4d, 5s and 5p subshells using the term-dependent Hartree-Fock wave functions.

In this paper we use our recently developed RPAE methods to study the photoionization of the I^+ ion. The difference between the current calculation and the previous RPAE calculations [9, 12-13] is that the photoionization cross section for each term of the I^+ ground state, I^+ 4d¹⁰5s²5p⁴ (³P), (¹D), (¹S)

has been calculated separately with the inclusion of all the inter-shell coupling among the I^+ $4d$, $5s$ and $5p$ subshells and without making any of the approximations used in the previous RPAE calculations. The total cross section is evaluated as the weighted average sum of the cross sections for each term. Our maximum for the I^+ $4d$ giant resonance shows an excellent agreement with the recent measurement [14].

2 Theory

The RPAE equation and corresponding dipole and Coulomb matrix elements for an atom with an outer open-shell is given by Eq. (1) and Appendix A of Ref. [8]. The Coulomb interaction in Eq. (1) causes an electron to switch from l_2 to l_1 . Similar terms will be added in the calculations for the electron switching from l_1 to l_3 , or from l_2 to l_3 etc. of the state $|l_3^{n_3}[L_3S_3]l_1^{n_1}[L_1S_1]l_2^{n_2}[L_2S_2]LS >$.

The ground state of the I^+ atom has the configuration $4d^{10}5s^25p^4(^3P, ^1D, ^1S)$. Therefore our calculations have three parts, each calculating one term of the ground state.

The following scattering processes are for the I^+ $4d^{10}5s^25p^4(^3P)$ term:

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^95s^25p^4(^3P)(^2D, ^2F, ^4D, ^4F)\epsilon f(^3P)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^95s^25p^4(^3P)(^2P, ^2D, ^2F, ^4P, ^4D, ^4F)\epsilon f(^3D)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^95s^25p^4(^3P)(^2F, ^4F)\epsilon f(^3S)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^{10}5s^25p^3(^2D)\epsilon s(^3D)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^{10}5s^25p^3(^2P)\epsilon s(^3P)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^{10}5s^25p^3(^4S)\epsilon s(^3S)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^{10}5s^25p^3(^2P, ^2D)\epsilon d(^3D)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^{10}5s^25p^3(^2P, ^2D)\epsilon d(^3P)$$

$$h\nu + 4d^{10}5s^25p^4(^3P) \rightarrow 4d^{10}5s^25p^3(^2D)\epsilon d(^3S)$$

$$\begin{aligned}
h\nu + 4d^{10}5s^25p^4(^3P) &\rightarrow 4d^{10}5s^25p^3(^4S)\epsilon d(^3D) \\
h\nu + 4d^{10}5s^25p^4(^3P) &\rightarrow 4d^{10}5s5p^4(^3P)(^2P, ^4P)\epsilon p(^3S) \\
h\nu + 4d^{10}5s^25p^4(^3P) &\rightarrow 4d^{10}5s5p^4(^3P)(^2P, ^4P)\epsilon p(^3P) \\
h\nu + 4d^{10}5s^25p^4(^3P) &\rightarrow 4d^{10}5s5p^4(^3P)(^2P, ^4P)\epsilon p(^3D) \\
h\nu + 4d^{10}5s^25p^4(^3P) &\rightarrow 4d^95s^25p^4(^3P)(^2D, ^2F, ^2P, ^4D, ^4F, ^4P)\epsilon p(^3D) \\
h\nu + 4d^{10}5s^25p^4(^3P) &\rightarrow 4d^95s^25p^4(^3P)(^2P, ^4P, ^2D, ^4D)\epsilon p(^3P) \\
h\nu + 4d^{10}5s^25p^4(^3P) &\rightarrow 4d^95s^25p^4(^3P)(^2P, ^4P)\epsilon p(^3S)
\end{aligned}$$

The total of 13 (3P), 18 (3D), and 8 (3S) final states have been included in the calculation.

The following scattering processes are for the $I^+ 4d^{10}5s^25p^4(^1D)$ term:

$$\begin{aligned}
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^95s^25p^4(^1D)(^2D, ^2F, ^2G)\epsilon f(^1P) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^95s^25p^4(^1D)(^2P, ^2D, ^2F, ^2G)\epsilon f(^1D) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^95s^25p^4(^1D)(^2S, ^2P, ^2D, ^2F, ^2G)\epsilon f(^1F) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^{10}5s^25p^3(^2P)\epsilon s(^1P) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^{10}5s^25p^3(^2D)\epsilon s(^1D) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^{10}5s^25p^3(^2P, ^2D)\epsilon d(^1P) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^{10}5s^25p^3(^2P, ^2D)\epsilon d(^1D) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^{10}5s^25p^3(^2P, ^2D)\epsilon d(^1F) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^{10}5s5p^4(^1D)(^2D)\epsilon p(^1D, ^1P, ^1F) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^95s^25p^4(^1D)(^2D, ^2F, ^2P)\epsilon p(^1D) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^95s^25p^4(^1D)(^2P, ^2D, ^2S)\epsilon p(^1P) \\
h\nu + 4d^{10}5s^25p^4(^1D) &\rightarrow 4d^95s^25p^4(^1D)(^2D, ^2F, ^2G)\epsilon p(^1F)
\end{aligned}$$

The total of 10 (1P), 11 (1D), and 11 (1F) final states have been included in the calculation.

The following scattering processes are for the $I^+ 4d^{10}5s^25p^4(^1S)$ term:

$$h\nu + 4d^{10}5s^25p^4(^1S) \rightarrow 4d^95s^25p^4(^1S)(^2D)\epsilon f(^1P)$$

$$h\nu + 4d^{10}5s^25p^4(^1S) \rightarrow 4d^{10}5s^25p^3(^2P)\epsilon s(^1P)$$

$$h\nu + 4d^{10}5s^25p^4(^1S) \rightarrow 4d^{10}5s^25p^3(^2P)\epsilon d(^1P)$$

$$h\nu + 4d^{10}5s^25p^4(^1S) \rightarrow 4d^{10}5s5p^4(^1S)(^2S)\epsilon p(^1P)$$

$$h\nu + 4d^{10}5s^25p^4(^1S) \rightarrow 4d^95s^25p^4(^1S)(^2D)\epsilon p(^1P)$$

A total of 5 (1P) final states have been included in the calculation.

The I^+ ground state and the core wave functions were obtained through the self-consistent Hartree-Fock (HF) calculation. Then the radial functions of the continuum electron were obtained by solving the linear HF equations without self-consistency using those core wave functions. Each channel includes three discrete and twenty continuum wave functions. Each radial part of the wave function was represented by 2000 points.

After evaluating the dipole and Coulomb matrix elements, the RPAE equation was solved for the partial cross sections for the 3P , 3D , 3S , 1P , 1D , and 1F final states. Then the photoionization cross sections for each term, 3P , 1D and 1S was obtained from the sum of the partial cross sections. Finally the total photoionization cross section was evaluated as the weighted average of each term.

3 Results

The $I^+ 4d - \epsilon f$ photoionization cross section is given in Fig.1. Dotted, dashed and dash-dot curves represent, respectively the photoionization cross sections from the term, $4d^{10}5s^25p^4(^3P)$, (^1S) and (^1D) . The three curves are very close to each other. Fig. 1. shows a broad region corresponding to the $4d - \epsilon f$ giant resonance. It is a shape resonance which is mainly determined by the potential shape. Fig. 1. gives a maximum cross section of 20.64 MB at the photon energy of 90.24 eV. Since almost all of the $4d - \epsilon f$ transition will emit a electron through

double Auger decay, this data should be compared with the experimental data for the I^{+3} ion.

Fig. 2. shows the $4d - \epsilon p$ photoionization cross sections. Obviously, the $4d - \epsilon p$ cross sections are much smaller in comparison than those for the $4d - \epsilon f$ transition. The description of the curves is the same as that in Fig. 1. At about 67 eV, which is near the 4d threshold the curve has a peak. Then, the cross section gradually decreases as the energy increases. Around 90 eV all three curves have a very small broadened peak. This is caused by the inter-shell coupling with the $4d - \epsilon f$ channel. After carefully analyzing the partial cross sections, we found that for the ground state term $4d^{10}5s^25p^4(^3P)$ the largest contribution to the cross section is from the transition to the final state 3D . However, for the term $4d^{10}5s^25p^4(^1D)$ the largest contributor to the cross section comes from the final state 1F .

The photoionization cross sections for the $5p$ and $5s$ subshells are given, respectively in Fig. 3 and Fig. 4. Fig. 3 demonstrates the $5p - \epsilon d, \epsilon s$ photoionization results. At about 19.38 eV the cross section is 17.89 MB. Then the cross section decreases as the energy increases. At 62.65 eV the cross section has reduced to 0.44 MB. After entering the energy range of the 4d giant resonance the cross section increases and reaches a maximum. A similar situation applies to the $5s$ photoionization process. However, firstly the cross section increases as the energy increases. Secondly, when the energy region of the 4d giant resonance is entered, the cross section increases sharply because of the inter-shell coupling with the $4d - \epsilon f$ channel.

Fig. 5. shows the total photoionization cross section, which is equal to the sum of the $4d - \epsilon f$, $4d - \epsilon p$, $5s - \epsilon p$, and $5p - \epsilon d, \epsilon s$ cross sections. In Fig. 5 the solid curve represents our average of three terms, $4d^{10}5s^25p^4(^3P, ^1D, ^1S)$. The dashed curve is from reference [10] using the time-dependent local-density spin approximation with an optimized effective potential and self-interaction correction (TDLSDA/OEP-SIC). The dotted curve is the experimental data [14], and the dash-dot curve demonstrates the previous RPAE calculation [13]. Our result shows a maximum of 23.12 MB at 90.24 eV, which is in excellent

agreement with the recent experimental result, 23(3) MB at 90 eV [14].

In conclusion, we used our recently developed RPAE method to study the photoionization cross sections of the I^+ ion with inclusion of all the inter-shell coupling among the $4d$, $5s$, and $5p$ subshells. We obtained, for the first time the photoionization cross sections for each term of the I^+ ground state. Our maximum cross section for the I^+ $4d$ giant resonance, 23.12 MB at the photon energy of 90.24 eV is in excellent agreement with the experimental data, 23(3)MB at 90 eV.

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References

1. M. Sano *et al*, J. Phys. B **29**, 5305 (1996).
2. E. D. Emmons *et al*, Phys. Rev. A **71**, 042704 (2005)
3. T. Koizumi *et al*, Physica Scripta **T73**, 131 (1997).
4. N. Watanabe *et al*, J. Phys. B:At. Mol. Opt. Phys. **31**, 4137 (1998).
5. Y. Itoh *et al*, J. Phys. B:At. Mol. Opt. Phys. **34**, 3493 (2001).
6. P. Andersen, T. Andersen, F. Folkmann, V. K. Ivanov, H. Kjeldsen and J. B. West, J. Phys. B:At. Mol. Opt. Phys. **34**, 2009 (2001).
7. A. Aguilar *et al*, Phys. Rev. A **73**, 032717 (2006).
8. Zhifan Chen and A. Z. Msezane, J. Phys. B: At. Mol. Opt. Phys. **39**, 4355 (2006).
9. M. Ya. Amusia, N. A. Cherepkov, L. V. Chernysheva and S. T. Manson, J. Phys. B:At.Mol.Opt.Phys. **33**, L37-32 (2000)
10. A. T. Domondon and X. M. Tong, Phys. Rev. A **65**, 032718 (2002).

11. G. O’Sullivan, C. McGuinness, J. T. Costello, E. T. Kennedy, and B. Weinmann, Phys. Rev. A **53**, 3211 (1996).
12. M. Ya. Amusia, N. A. Cherepkov, L. V. Chernysheva, and S. T. Manson, Phys. Rev. A **61**, 020701(R) (2000)
13. M. Ya. Amusia, L. V. Chernysheva, V. K. Ivanov, and S. T. Manson, Phys. Rev. A **65**, 032714 (2002).
14. H. Kjeldsen, P. Andersen, F. Folkmann, H. Knudsen, B. Kristensen, J. B. West, and T. Andersen, Phys. Rev. A **62**, 020702 (2000).
15. L. Nahon, A. Svensson, and P. Morin, Phys. Rev. A **43**, 2328 (1991).
16. Zhifan Chen and A. Z. Msezane, Phys. Rev. A, **77**, 042703 (2008).

Figure Captions

Fig. 1. Photoionization cross section for the $I^+ 4d - \epsilon f$ for the ground state terms of (3P , 1D , 1S). Dotted, dashed and dash-dot curves represent, respectively the results for 3P , 1D and 1S .

Fig. 2. Curves have the same meaning as those in Fig. 1, except that they demonstrate the $I^+ 4d - \epsilon p$ photoionization cross section.

Fig. 3. Curves have the same meaning as those in Fig. 1, except that they demonstrate the $I^+ 5p$ photoionization cross section.

Fig. 4. Curves have the same meaning as those in Fig. 1, except that they demonstrate the $I^+ 5s$ photoionization cross section.

Fig. 5. Total cross sections for the I^+ photoionization in the energy region of $4d - \epsilon f$ giant resonance versus photon energy (eV). Solid curve is from our average cross sections for the terms (3P), (1D), and (1S), dotted curve represents the experimental data, dashed curve shows the calculated result from reference [10], and the dash-dot curve is from the calculation of Amusia et al [13].









